Physics-Informed Neural Networks for Contaminant Transport in Aquifers

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Abstract

This report summarizes recent progress on simplified baseline and parametric Physics-Informed Neural Networks (PINNs) for the 1D advection-dispersion equation in a fully dimensionless form. The baseline model solves for C* as a function of (x*, t*), while the parametric model extends the input space to (x*, t*, log Pe) to cover a wide Peclet range. Results are presented as dimensionless concentration profiles and loss curves, with an analytical overlay used strictly as a qualitative shape reference.

1 Executive Summary

The baseline PINN has been simplified into a linear, step-by-step implementation, and the parametric PINN now generalizes across multiple Peclet numbers within a single model. Both scripts operate entirely in dimensionless variables. Key outcomes include stable training behavior and consistent qualitative trends across Pe. The two scripts referenced in this report are the simplified baseline PINN and the parametric PINN.

2 Scope

This report focuses on a dimensionless formulation of the 1D advection-dispersion equation with inputs x*, t*, and log Pe. Emphasis is placed on clarity, reproducibility, and parametric generalization rather than architectural complexity.

3 Methods

3.1 Dimensionless problem

The governing equation is:

$$C^*_{t^*} + C^*_{x^*} - \frac{1}{Pe} C^*_{x^* x^*} = 0$$

with domain x* in [0, 1], t* in [0, t*$_{f}inal], and Pe in [Pe_m in, Pe_m ax]. Initial and boundary conditions are C*$ $(x*, 0) = 0, C*(0, t*) = 1, and C*(1, t*) = 0.$

3.2 Baseline PINN

The baseline model maps (x*, t*) to C* and is trained using a weighted loss that combines PDE residual, initial condition, inlet, and outlet boundary losses. Collocation points are sampled uniformly within the dimensionless domain.

3.3 Parametric PINN

The parametric model augments the input with log Pe, allowing a single network to represent solution behavior across a wide Peclet range. Sampling is uniform in log Pe to balance coverage across orders of magnitude.

3.4 Analytical overlay

Analytical curves are overlaid as a qualitative shape reference using a dimensionless proxy mapping (U = 1, C0 = 1, D = 1/Pe). This overlay is not treated as a strict benchmark.

4 Results

4.1 Baseline PINN

Figure **??** shows the baseline loss curves. Figure **??** shows C* profiles over x* at selected t* values.

`baseline_loss.pdf`

Figure 1: Baseline PINN loss curves (dimensionless).

`baseline_profiles.pdf`

Figure 2: Baseline PINN C* profiles over x* at selected t* values with analytical overlay (shape reference).

4.2 Parametric PINN

Figure **??** shows the parametric training losses. Figures **??** and **??** illustrate C* profiles for two representative Peclet numbers. As expected, low Pe yields smoother diffusion-dominated profiles, while high Pe produces sharper fronts.

parametric_loss.pdf

Figure 3: Parametric PINN loss curves (dimensionless).

5 Summary and Next Steps

The baseline PINN is simplified and stable, and the parametric PINN demonstrates consistent qualitative behavior across Peclet numbers in a fully dimensionless setting. Next steps include sensitivity checks on t*$_{f}inal, optionallossreweighting, andexpandingthesetofreportedPevaluesforvisualcoverage.$

parametric_profiles_pe10.pdf

Figure 4: Parametric PINN C* profiles for Pe = 10.

parametric_profiles_pe1e5.pdf

Figure 5: Parametric PINN C* profiles for Pe = 1e5.